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MCNPX, VERSION 2.5.e

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ABSTRACT

MCNPX is a Fortran90 Monte Carlo radiation transport computer code that transports all particles at all energies. It is a superset of MCNP4C3 and has many capabilities beyond MCNP4C3. These capabilities are summarized in this report, along with the MCNPX quality guarantee and code availability. In addition, the new capabilities of the latest version, MCNPX 2.5.e, are described.

1.0. INTRODUCTION

MCNPX (MCNP eXtended) is a Fortran90 (F90) Monte Carlo radiation transport computer code that transports all particles at all energies. It is a superset of MCNP4C3 and has many capabilities beyond MCNP4C3. MCNPX is a production computer code for modeling the interaction of radiation with matter, and its quality is guaranteed; it can be used with confidence. MCNPX is available from the Radiation Safety Information and Computational Center (RSICC, http://www-rsicc.ornl.gov) and the Office of Economic Community Development (OECD)/Nuclear Energy Agency (NEA) (http://www.nea.fr). For approved users, beta test program versions may be downloaded from the MCNPX website at http://mcnpx.lanl.gov/.

1.1. New MCNPX 2.5.e Capabilities

MCNPX 2.5.e offers many new capabilities. The complete summary of MCNPX capabilities beyond MCNPX 2.3.0 and MCNP4C is provided in the MCNPX features list available on the MCNPX website at http://mcnpx.lanl.gov/. The new capabilities and enhancements of MCNPX 2.5.e beyond MCNPX 2.5.d are listed as follows (where applicable, the initials of the principal developers are shown in parentheses).*

- Two-dimensional (2D) color tally contour plots, including lattices and radiography (GWM)
- Significant speedup of criticality problems run in parallel with MPI (GWM/NAC)
- 64-bit integer support—MCNPX can now run trillions of histories (GWM)
- NAG/IBM/INTEL compiler extensions—MCNPX runs on a Macintosh G5 (GWM/TLR)
- Photon Doppler broadening (from MCNP5) (AS)
- Significant improvements in
    - INCL4/ABLA—more robust with increased precision (JSH/GWM/JCD)
    - photonuclear model physics (FXG)

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  - o coincidence capture tallies (MTS/JSH)
  - o S (α, β) thermal treatment (RCL/EJP)
- corrections/enhancements/extensions.

1.2. Guarantee

MCNPX is guaranteed. We are so confident of the quality of MCNPX that we will pay $20 to the first person finding anything that does not meet or exceed the capabilities of MCNPX 2.3.0 and MCNP4C3. We also will pay a brand new $2 bill for any error in MCNPX that has been inherited from its constituent codes.*

MCNPX is a better quality code than MCNP4C3. First, it corrects many MCNP4C3 problems. Second, cash awards have been earned less frequently with MCNPX than with MCNP4C3 and its predecessors, and most of those awards have been given for problems carrying over from older code versions; very few errors have been found in the new MCNPX versions. A listing of winners is available at http://mcnpx.lanl.gov/. MCNPX bugs are described in the release notes for each MCNPX version.

1.3. Availability

MCNPX 2.4.0 is available from the RSICC in Oak Ridge, Tennessee, USA, at http://www-rsicc.ornl.gov/. MCNPX 2.4.0 is also available from the OECD NEA Data Bank in Paris, France, at http://www.nea.fr/.

An essential part of the MCNPX software quality assurance plan is the beta test program. Before a code version goes to RSICC or OECD/NEA, it is made available to more than 1000 MCNPX beta testers worldwide. MCNPX 2.5.e is available to beta testers on the MCNPX website at http://mcnpx.lanl.gov/. To apply for a beta test password and have access to the latest MCNPX versions, contact Laurie Waters at lsw@lanl.gov.

All beta test, RSICC, and OECD/NEA versions of MCNPX are guaranteed with cash awards.

2.0. DESCRIPTION OF NEW MCNPX 2.5.e FEATURES

The principal new capabilities of MCNPX 2.5.e are

- 2D color tally contour plots (GWM)
- MPI speedup for criticality calculations (GWM/NAC)
- 64-bit integer support (GWM)
- NAG/IBM/INTEL compiler extensions (GWM/TLR)
- photon Doppler broadening (from MCNP5) (AS)

* Cash Award Fine Print: This offer is subject to cancellation or modification without notice. A bug is defined as an error we choose to correct in the source code. We make awards even for the most trivial or insignificant of problems, but not for proposed code enhancements or proposed extended capabilities. Awards are given only to the first MCNPX user reporting a problem. Reported problems must be reproducible, and awards are paid when the correction is integrated into a forthcoming MCNPX version. We endeavor to make MCNPX the most error-free and robust Monte Carlo radiation transport code possible, and we back this code with a cash guarantee.

2.1. Color Contour Tally Plots

Tally output now may be plotted as 2D color contours from either MCTAL or RUNTPE files. For example, a radiography tally with s and t axes specified on FS and C cards can be plotted with the MCNPX Z option, as illustrated in the following example. For the first time, the “i” and “j” indices of i,j,k lattice tally plots also can have contour plots. We will extend the capability to mesh tally plots in a future MCNPX version.

2.1.1. Example

The following example is a radiograph of a 4-cm-radius, 1-cm-thick ^{238}U disc with an embedded 2-mm-void sphere. The input file is

```
Radiography Tally
1 5 -25.0  -1 3          imp:p=1
2 0         (1:-3) –2    imp:p=1
3 0         2            imp:p=0

1 RCC 0 0 0  0 0 1  4
2 RPP -1000 1000 -1000 1000 -1000 1000
3 SPH 2 0 1  .2

mode p
nps 100000 5
sdef pos=0 0 -20 axs=0 0 1 rad=d1 ext=0 vec=0 0 1 dir=d2 erg=6
si1 0 .1
sp1 -21 1
si2 -1 1
sp2 -31 1
m5 92238 1
print
prdmp 2j 1
tir5:p 0 0 10 0 0 0 -100 0 100 0
fs5    -10. 99i 10.
c5     -10. 99i 10.
```

To get the contour plot,

MCNPX Z RUNTPE=*filename*

is run.

The contour plots also may be read from a MCTAL file instead of the RUNTPE. When the code gives the MCPLOT prompt, two dimensions must be entered with the free command; for example, S and C, as

MCPLOT> free SC .

Recall that the tally dimensions are

F	=	surface / cell / detector F card bin,
D	=	total / direct or flagged bin,
U	=	user bin,
S	=	segment or radiography s-axis bin,
M	=	multiplier bin,
C	=	cosine or radiography t-axis bin,
E	=	energy bin, and
T	=	time bin.

The results are provided in Fig. 1.

Although the picture is striking, the embedded void sphere is not seen and the shapes in the symmetrical disc indicate poor convergence. In a direct tally (MCPLOT command: fixed D 2), the embedded sphere is seen, but the picture is rather plain.

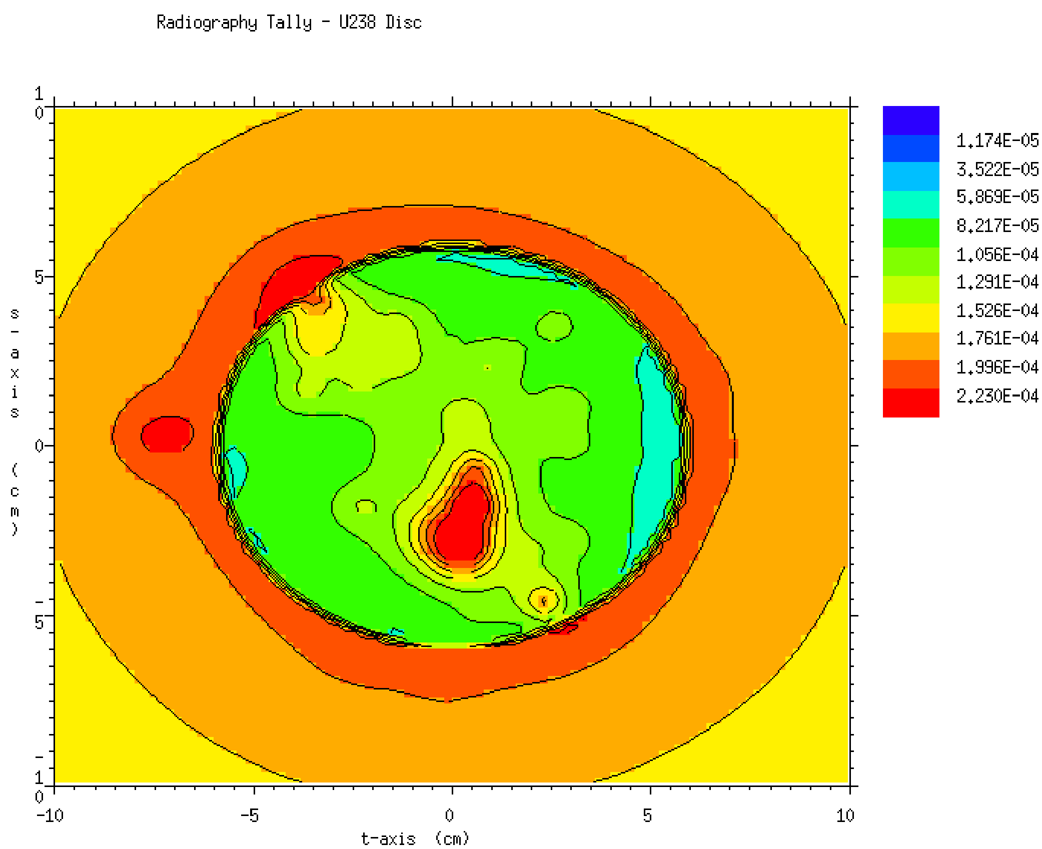

Fig. 1. Scattered photon radiographic image of a ^{238}U disc.

2.1.2. User Interface

2.1.2.1. MCPLOT FREE Command. The MCPLOT free command works the same as always, but with the following extension:

FREE X[Y] [nxm] [all] .

Variables x and y are tally bin indices (fdusmcet) or lattice indices (ijk) for lattice tally plots. Currently, the lattice indices are limited to "i" or "ij" and the other indices are specified using the "fix" command (see the following examples). Specifying a single variable after the free command produces a 1D plot. Specifying two variables produces a 2D contour plot. The remaining two keywords are valid only when x = i or xy = ij. The "nxm" keyword specifies the number of bins associated with the "i" and "j" lattice indices. The "all" keyword specifies that the minimum and maximum contour range should be taken from all of the tally bins. Omitting this keyword results in defaulting to the minimum and maximum contour range, which includes only those tally values contained in the specified 2D plot.

Example 1:

free i 64x64 fix j=38 fix k=30

This command specifies a 1D lattice tally plot of the cell bins, which should correspond to a lattice tally with 64 "i" index bins, 64 "j" index bins, and at least 30 "k" index bins. With the "k" index set to 30 and the "j" index to 38, the offset into the f bins will be $29 \times 64 \times 64 + 37 \times 64 = 121152$. The minimum and maximum values will be determined from the 64 "i" bin values included in the plot. If the "j" and "k" indices are not specified, their default value of 1 is assumed, which results in an offset of 0.

Example 2:

free ij 10x30 all fix k=60

This example specifies a 10 x 30 2D contour plot, which should correspond to a lattice tally with 10 "i" bins, 30 "j" bins, and at least 60 "k" bins. Note that the "k" index is specified using the "fix" command, which sets the offset into the f bins as $60 \times 10 \times 30 = 18000$. In this case, the contour range is taken from all of the f-bin tally values.

2.1.2.2. MCPLOT FIXED Command. The MCPLOT FIX command works the same as always, but has the following extension:

fix x=n

The keyword "x" is one of the same tally bin indices (fdusmcet) as before. Or it may now be one of the lattice indices (ijk) for lattice tally plots. The value of "n" specifies a bin value for that index. Currently, only the "j" and "k" indices are allowed for a 1D ijk plot, and only the "k" index is allowed for a 2D ijk contour plot.

2.1.2.3. MCPLOT CONTOUR Command. The MCPLOT CONTOUR command has an additional optional keyword. The form is now

Contour cmin cmax cstep [%] [noline] .

The default contour plot will include black lines separating the contour colors. The lines can be turned off with the new "noline" keyword. The MCNP commands cmin, cmax, and cstep are the minimum, maximum, and step values for contours. The "%" will cause these to be interpreted as percentages. The default is 5 95 10 %.

2.1.3. Future Work

The future work is as follows:

1. Extend 2D color tally contour plots to mesh tallies.

2. Subblocking (i.e., plotting subsections of the full contour plot) is performed with a standard contour plot; however, this capability currently is disabled for specialized contour plots (i.e., free ij). The only drawback is that larger arrays are required to store the tally values (these arrays can be quite large for a detailed contour plot, e.g., 1000 × 1000). To allow subblocking, additional logic is required in PLOTCN to subblock on a full horizontal row at a time.

3. This contour upgrade allows for easy viewing of lattice tally data, but it is limited to look at 2D slices in only one way for a full 3D lattice. In this case, plots can be only in the "i" and "j" index plane, with "k" slices specified with the "fix" command. A user currently cannot look at a "j" and "k" contour plot or an "i" and "k" contour plot. To allow this, significant changes are required to be made to subroutine EXTRCT that would enable the extraction of noncontiguous tally values.

2.2. MPI Speedup of Criticality Calculations

Note: This new capability speeds up MPI KCODE calculations but also has some collateral consequences for sequential KCODE calculations (see Section 2.2.1).

Criticality calculations (KCODE source) *will now run 10 to 1000 times faster* in parallel with MPI multiprocessing. The speedup depends on the number of CPUs and the number of histories per cycle. As the number of CPUs increases above ~8 and the histories per cycle approach ~1M, the speedup quickly increases from a factor of ~10 to >1000 with 64 CPUs.

The speedup has been achieved by having the next-generation fission source points on each processor remain on that processor. No longer are the fission source points from all processors combined at the end of each cycle for rebroadcasting in the next cycle. The considerable expense of grouping the particles together at each processor rendezvous has been eliminated. The method was developed by Nate A. Carstens (MIT) and Gregg W. McKinney (LANL, D-5).

2.2.1. DXTRAN and Detector Tracking Differences

All calculations with DXTRAN and detectors—not just KCODE or parallel calculations—generally do not track any longer. Answers are still correct, but these next-event estimator problems do not track unless the twenty-first entry on the DBCN card is set nonzero or the default Russian roulette detector game (DD card) is not played. The tracking difference occurs because the default Russian roulette game no longer adjusts the roulette criteria at the 200th history. The Russian roulette criteria still are set at all tally fluctuation chart intervals, NPD, the fifth entry on the PRDMP card. The default for NPD is still 1000 histories for fixed-source problems, but it is now NPD = 1 (at the end of each cycle) for KCODE problems. Thus, a fixed-source problem that used to start playing Russian roulette on next-event estimates at history 200 now waits until history 1000.

2.2.2. User Interface Changes for Both Sequential and Parallel KCODE Problems

The new method has consequences for both sequential and parallel KCODE calculations:

- Tally fluctuation charts are printed only at the ends of KCODE cycles rather than at specific particle intervals.
- The fifth entry of the PRDMP card is changed for KCODE calculations. The fifth entry is NPD, the tally fluctuation chart print interval. For KCODE calculations, NPD is now the number of cycles (default = 1).
- KCODE problems with DXTRAN and point detectors are still correct but may not track previous versions if the default Russian roulette game on small scores is played. The tracking difference occurs because the roulette criteria are updated in different places. DXTRAN and detectors utilizing negative DD card entries (to have a constant Russian roulette game criteria) still track.
- Setting the twenty-first entry on the DBCN card to 1 will cause MCNPX to track MCNPX 2.5.d without the new speedup capability:

```
DBCN  20J     1
```

2.2.3. User Interface Changes for Parallel KCODE Problems

The user interface changes are the following.

- The KCODE speedup is available only for negative JTASKS: tasks = -n x m on the MCNPX execution line. Microtasking/load balancing (positive JTASKS) calculations use the slower, former MCNP4C communication algorithm for KCODE source updating. A warning is issued if JTASKS > 0 in a KCODE calculation.
- In rare cases, a subtask may deplete its source particles. Only problem efficiency is affected, and a warning is issued.

2.2.4. Compiler and Operating System Problems for Parallel KCODE Calculations

The compiler and operating system problems are the following.

- "CTRL-C" and "quit" on a multiple-processor MPI run in Linux do not finish writing the OUTP file before MCNPX exits. This failure appears to be an MPI error (possibly a feature) in the MPI_FINALIZE call, where the last processor kills all subtasks and the master.

- CTRL-C interrupt does not function properly in Windows 2000 (probably general to all Windows). The user can attempt to quit, but MCNPX will hang and the user will be forced to kill the process through multiple CTRL-C commands.

- The Portland Group pgcc compiler (Version 4.02) will not compile the ANL mpich-1.2.5 properly on a Linux system. However, GCC 3.2.3 will work to build the MPICH libraries.

2.3. 64-Bit Integer Support

MCNPX has been restructured to enable 64-bit integers. MCNP and MCNPX always have had 64-bit floating-point real integers either by use of compiler directives on supercomputers or by double precision on "cheap" computers (most systems). However, the integers have been 4 byte (32 bit) on all but a few supercomputers, which limits the number of histories that can be run to about 2 billion. It also limits the number of cross sections and tallies in a problem because these use integer pointers.

With the 64-bit integer capability, up to 1×10^{18} histories can be run. Memory access problems can be avoided and still have almost endless cross sections and tallies.

The print field for the number of histories run in a problem has been increased to 12 digits to accommodate the long runs now possible with parallel processing.

2.3.1. Recompilation Requirements for 64-Bit Integers

The default for MCNPX is still 4-byte integers. The executable versions provided on the MCNPX Beta Test page are all 4-byte integer versions. To use the 64-bit version, users must

1. recompile with special options, and

2. either use type-1 ascii cross-section tables or rebuild their type-2 binary cross-section tables using 64-bit integer pointers with MAKXS.

If users generally recompile their own MCNPX versions and use type-1 ascii cross sections, they can go to the 64-bit integers rather easily. When the users configure, they can simply add the directives

```
--with-FFLAGS=-i8   –with-NOCHEAP
```

The "with-NOCHEAP" directive is not available on all systems. If it is not recognized on the users' systems, then the compile directive

```
--with-FFLAGS=-i8
```

must be added and

–DCHEAP=1

must be removed from src/mcnpx/mcnpf/Makefile.h.

The 64-bit integer capability is unavailable on PCs. The –i8 compile option is not available on the CVF F90 compiler and possibly other compilers. The 64-bit integers will increase the size of the code.

2.3.2. Additional Notes

The 64-bit integer capability was an extensive change to MCNPX because it affected most F90 “kind” specifications. We also eliminated all “REAL” declarations where floating-point variables went to different default (usually 32-bit) lengths on various systems. A consequence is that real variables are all 64-bit, unless some other length is required for interfaces to plotting, interrupts, or other special purposes. The tracking between different compilers and platforms is now more consistent. Finally, this capability made extension to new compilers and platforms (see Section 2.4) easier.

2.4. NAG/IBM/INTEL F90 and Compiler Extensions

MCNPX now runs on a greater variety of platforms and operating systems by utilizing more standard F90 constructs and some fairly extensive code and autoconfiguration changes. In particular, MCNPX runs on the G5 OS X system using the NAG 4.2 compiler for the Apple Power Mac G5. MCNPX 2.5.e also runs on the Apple Power Mac G5 with the IBM compiler.

The NAG compiler passes the Silicon Graphics, Inc. (SGI) test suite on the Mac with “-O1” optimization. The IBM compiler passes with “-O2” optimization and is 17% faster. A trial version of the IBM compiler is available from http://www.ibm.com/; see “support & downloads—trials & betas A-Z—XL Fortran.”

No MCNPX parallel capability has yet been developed for the NAG compiler.

2.5. Photon Doppler Broadening

The MCNP5 photon Doppler broadening capability[*] developed by Avneet Sood is now available in MCNPX. Unlike MCNP5, the default is “off” (PHYS:P 4j 1) because the effect is small but time-consuming.

The electron binding effect on a scattered photon’s energy distribution appears as a broadening of the energy spectrum due to the precollision momentum of the electron. The effect applies to incoherent scatter (Compton scatter). The scattered energy of a Doppler-broadened photon is

[*] X-5 Monte Carlo Team, “MCNP—A General Monte Carlo N-Particle Transport Code, Version 5, Volume II: User’s Guide,” Los Alamos National Laboratory report LA-CP-03-0245 (April 24, 2003), p. 2-59.

calculated by selecting an orbital shell, sampling the projected momentum from the Compton profile, and then calculating the scattered photon energy.

2.5.1. Photon-Doppler-Broadening Physics

Two research notes on photon Doppler broadening are (or soon will be) available on the MCNPX WWW site, http://mcnpx.lanl.gov/documents/. The following quote is taken from the first research note, X-5:AS-02-16:

> Incoherent scattering of an incident photon can occur with a bound electron in a shell of a material and will generate a Compton electron and a scattered photon. The electron binding effects become important when the incident photon energy is near a few hundred keV. The result of the binding effects on the angle and energy of the scattered photon must be taken into account for accurate simulation of low-energy photon transport. The effect of the bound electron on the scattered photon's angular distribution appears as a reduction in the total scattering cross section in the forward direction. MCNP currently accounts for the electron binding effects on the angular distribution of the scattered photon by modifying the Klein-Nishina differential cross section with a form factor. The electron binding effect on the scattered photon's energy distribution appears as a broadening of the energy spectrum due to the precollision momentum of the electron. This effect on the energy distribution of the incoherently scattered photon is called Doppler broadening.

2.5.2. User Interface

Photon Doppler broadening is controlled by the fifth entry on the PHYS:P card as

```
PHYS:P    EMCPF    IDES  NOCOH    ISPN  NODOP
```

where

EMCPF = upper energy for detailed physics (default = 100 MeV)

IDES = generate electrons by mode E or thick-target-bremsstrahlung (default = 0 = on)

NOCOH = coherent (Thomson) scattering (default = 0 = on)

ISPN = -1/0/1 = analog/off/biased. The bias causes a photonuclear event at each photoatomic event. (default = 0 = off)

NODOP = 0/1 = on/off Doppler energy broadening. (default = 1 = off)

Turning on photon Doppler broadening (NODOP = 0) has no effect unless photon-Doppler-broadening momentum profile data are available in the photon library. These data are available in the MCPLIB03 and MCPLIB04 photon libraries with ZAID identifiers .03p and .04p.

3.0. MCNPX 2.5.e FEATURE EXTENSIONS AND ENHANCEMENTS

Several MCNPX features have been extended and have included changes or additions to the user interface.

3.1. FT8 Capture Tally

The coincidence capture capability of MCNPX has been upgraded as follows:

- Spontaneous fission with multiplicity zero now contributes to the zero capture entry in the coincidence capture tally.
- Factorial moments now include contributions from all captures, not just up to maximum, and include contributions to the moments from zero fission multiplicity.
- The maximum number of moments and captures may be user-specified.

3.1.1. Increasing the Default Number of Captures and Moments

The maximum number of captures and moments now may be specified on the FT8 card:

FT8 -Mc -Mo I1 I2 …

where

Mc = maximum number of captures (default = 21)
Mo = maximum number of moments (default = 12).

3.1.2. Interpreting Capture Tally Output

The FT8 CAP coincidence capture tally option produces both a standard tally, which is generally unreadable, and a coincidence capture table, print table 118. An example is provided here to help in the interpretation of this table.

```
neutron captures, moments & multiplicity distributions. tally 8 print table
118

 cell:    999

 neutron captures on 3he
                     captures      captures    multiplicity fractions
         histories   by number     by weight    by number     by weight   error

 captures =  0     700       0   0.00000E+00  7.00000E-02  3.25400E-02  0.0364
 captures =  1    2285    2285   1.06220E-01  2.28500E-01  1.06220E-01  0.0184
 captures =  2    3223    6446   2.99647E-01  3.22300E-01  1.49823E-01  0.0145
 captures =  3    2489    7467   3.47109E-01  2.48900E-01  1.15703E-01  0.0174
 captures =  4    1022    4088   1.90033E-01  1.02200E-01  4.75084E-02  0.0296
 captures =  5     209    1045   4.85775E-02  2.09000E-02  9.71551E-03  0.0684
 captures =  6      51     306   1.42246E-02  5.10000E-03  2.37077E-03  0.1397
 captures =  7      12      84   3.90480E-03  1.20000E-03  5.57828E-04  0.2885
```

```
 captures >  7       9      73   3.39345E-03  9.00000E-04  4.18371E-04  0.3332

    total        10000   21794   1.01311E+00  1.00000E+00  4.64857E-01  0.0056

      factorial moments             by number              by weight

             3he                2.17940E+00 0.0056      1.01311E+00 0.0056
        3he(3he-1)/2!           2.01890E+00 0.0128      9.38499E-01 0.0128
     3he(3he-1)(3he-2)/3!       1.06390E+00 0.0291      4.94561E-01 0.0291
  3he(3he-1) .... (3he-3)/4!    3.93800E-01 0.0744      1.83061E-01 0.0744
  3he(3he-1) .... (3he-4)/5!    1.34100E-01 0.1636      6.23373E-02 0.1636
  3he(3he-1) .... (3he-5)/6!    4.43000E-02 0.2666      2.05932E-02 0.2666
  3he(3he-1) .... (3he-6)/7!    1.12000E-02 0.3808      5.20640E-03 0.3808
  3he(3he-1) .... (3he-7)/8!    1.70000E-03 0.5548      7.90257E-04 0.5548
```

The capture tally input for this problem was

F8:n	999				input F8 card
FT8	CAP	-8	-8	2003	input FT8 CAP card

Note that the line captures > 7 9 73 indicates that nine histories had eight or more neutrons captured. This implies that eight histories had 8 x 8 = 64 neutrons captured and one history had 1 x 9 neutrons captured for a total of 73 neutrons captured. The table of captures was evidently too short, and the problem should have been run with FT8 CAP -9 -9 or even more captures and moments. Only the "captures > 7" line and the error estimate on the totals capture line are affected; all other information is correct as if more captures and moments were listed.

The following information is an interpretation of the neutron captures on the ^{3}He table.

Column 1 is the number of histories according to the number of captures by the designated material (2003 = ^{3}He) in the designated cell (999). These values sum to the total number of source histories for the problem, nps = 10000.

Column 2 is the number of captures by 2003 in cell 999 = 21794. Because analog capture is the default for F8 tallies, the total weight captured is also 21794.0.

Column 3 is the total weight captured divided by the tally normalization. For SDEF PAR = -SF, the tally normalization equals the number of source histories, which equals the number of spontaneous fissions, which equals 10000. For SDEF PAR = -SF, column 3 would be 21794.0/10000 = 2.17940. In this problem, SDEF PAR = SF and the tally normalization is the source particles, which equals spontaneous fission neutrons, which equals 21512. Thus, captures by weight is 21794.0/21512 = 1.01311.

Column 4 is the multiplicity fraction by number, which is the value in column 1, divided by the number of source histories. The total is always 1.00000.

Column 5 is the multiplicity fraction by weight, which is the weight of histories undergoing capture, divided by the tally normalization. For SDEF PAR = -SF, this would be 10000.0/10000

= 1.00000. In this problem, SDEF PAR = SF and the multiplicity fraction by weight is 10000.0/21512 = 0.464857.

The interpretation of the factorial moments table now follows.

The first moment by number is the number of captures divided by the number of source histories = 21794/10000 = 2.17940.

The first moment by weight is the total weight of capture divided by the tally normalization. For SDEF PAR = -SF, this would be 21794.0/10000 = 21794.0. In this problem, SDEF PAR = SF and the first moment by weight is 21794.0/21512 = 1.01311.

The second moment is N*(N-1)/2, where N is the number of captures. In this problem,

N	N*(N-1)/2		histories		product
1	0	×	2285	=	0
2	1	×	3223	=	3223
3	3	×	2489	=	7467
4	6	×	1022	=	6132
5	10	×	209	=	2090
6	15	×	51	=	765
7	21	×	12	=	252
8	28	×	8	=	224
9	36	×	1	=	36
	sum			=	20189

The second moment by number is divided by the number of histories as

20189/10000 = 2.01890 .

Because of analog capture, the second moment weight is 20189.0. The second moment by weight is divided by the tally normalization. For SDEF PAR = -SF, this would be 20189.0/10000 = 2.01890, which is the same as the second moment by number. In this problem, SDEF PAR = SF and the second moment by weight is

20189.0/21512 = 0.938499 .

The seventh moment is

$7 \times 6 \times 5 \times 4 \times 3 \times 2 \times 1/7!$	=	1	×	12	=	12
$8 \times 7 \times 6 \times 5 \times 4 \times 3 \times 2/7!$	=	8	×	8	=	64
$9 \times 8 \times 7 \times 6 \times 5 \times 4 \times 3/7!$	=	36	×	1	=	36
sum					=	112

Thus, 112/10000 = 0.0112.

The eighth moment is

$8 \times 7 \times 6 \times 5 \times 4 \times 3 \times 2 \times 1/8!$	=	1	$\times$	8	=	8
$9 \times 8 \times 7 \times 6 \times 5 \times 4 \times 3 \times 2/8!$	=	9	$\times$	1	=	9
sum					=	17

Thus, 17/10000 = 0.0017.

The ninth moment is

$9 \times 8 \times 7 \times 6 \times 5 \times 4 \times 3 \times 2 \times 1/9!$	=	1	$\times$	1	=	1

Thus, 1/10000 = 0.0001.

3.2. Photonuclear Model Physics

Photonuclear physics models enable (γ,n) and other photonuclear reactions when photonuclear data tables are unavailable. Franz Gallmeier (ORNL) has upgraded the MCNPX 2.5.e CEM2k photonuclear model physics model to address requested improvements in the photoabsorption and photofission of actinides.

No change occurs in the user interface; the new gdr.dat file simply is obtained.

The new gdr.dat file (src/Data/CEM/gdr.dat in the MCNPX source file) has improved cross-section parameters (for photonuclear cross sections) that were obtained by fitting to the BOFOD photonuclear cross sections. It replaces the old gdr.dat file, which still can be read and will track as before.

The new MCNPX 2.5.e photonuclear physics model modifications adjust the photofission cross sections in CEM by the ratio of fission and neutron evaporation level density parameters (wam). For selected isotopes (implemented for ^{235}U and ^{232}Th), a list of energy-dependent wam parameters was generated that matched the fissility of the BOFOD photonuclear cross-section data. The list is entered into the code as data statements in the newly created subroutine set_wam.F, which provides a wam parameter for a requested nuclide “iza” at a incident photon energy of “t0mev” interpolating between two tabulated values. If data for a requested nuclide are not available, the code returns wam = 0.0. We hope to provide wam parameters for more isotopes in the future.

Photonuclear models are designed to work with the CEM2k physics package and are fragile or may not work with other packages.

3.3. INCL Enhancements

The INCL/ABLA physics package has been enhanced as follows.

- At low energies, the INCL Intranuclear Cascade can be switched to the Bertini model to increase speed.

- ABLA is now the default fission evaporation model for INCL.
- A warning is issued if ISABEL (LCA(3) = IEXISA > 0) is specified because INCL does not work with ISABEL.
- All INCL/ABLA variables now are double precision.
- The MCNPX random number generator is used for INCL/ABLA.
- Many corrections now make INCL/ABLA more robust and run faster, including the capability to not bank extremely low-energy particles.

3.4. Improved S(α,β) Treatment

The S(α,β) thermal neutron treatment in many cases uses discrete energies instead of 32-equiprobable-bin histogram energies. The result is nonphysical spikes in the thermal neutron spectrum. These spikes now are smoothed out by an algorithm provided by Robert Little and Eric Pitcher of LANL. MCNPX can still track the old algorithm by setting DBCN(21) = 1.

3.5. Additional Enhancements

The following enhancements were made to MCNPX 2.5.e in addition to the major new capabilities explained in Section 2.0. Only the first enhancement affects the user interface.

3.5.1. Detector/DXTRAN Underflow Control

DXTRAN and point detector contributions are based on the next-event estimator that makes contributions of

$$W * p(\mu)*\exp(\lambda) / 2\pi R^2 \quad ,$$

where

W = particle weight;

$p(\mu)$ = the density function for scattering to the detector or DXTRAN sphere;

R = the distance from collision to the detector or DXTRAN sphere; and

λ = the attenuation factor, namely the sum of total macroscopic cross section times the track length for each material region crossed between the collision and detector or DXTRAN sphere.

Currently, if $\lambda > 80$, then $\exp(\lambda) = 0$ and the score is terminated as “underflow in transmission.” These small contributions are truncated, or neglected, which biases answers by omitting them. Generally, these contributions are insignificant to the final answer. However, in some cases, the underflow contribution is significant and needed. And when DXTRAN spheres or point detectors are used to obtain tally contribution for generating weight windows, these underflow contributions occasionally cannot be neglected.

It is now possible to specify the underflow limit with the sixth entry on the DBCN card. The default is 80, but other values are now accepted.

If DXTRAN/detector underflow is significant in a calculation, serious problems generally arise, such as not sampling enough collisions near the detector. Changing the underflow limit should be done only with extreme caution.

3.5.2. Lattice Tally Initialization Speedup

Lattice tallies, which were significantly sped up in MCNPX 2.5.d, now also are sped up in the initialization phase of the code when the input is read in and processed. The speedup applies only to tallies in lattices where the full lattice at one universe level is specified in the tally and there is exactly one cell or lattice bin specified at each level above and below the full lattice.

3.5.3. New Proton Data Library Formats

Lithium-7 and other new proton data tables now can be read when they have multiple reaction channels. Until now, the MCNPX proton data tables worked only when one reaction channel existed. The coding has been generalized (with support from Robert Little, LANL, X-5) to handle multiple channels.

3.5.4. Geometry Plot Coloring by Negative Universe Number

If geometry plots are colored by universe number (U) and the universes are specified negative, the color of the absolute value of the universe is used. Negative universes may be specified on cell cards to speed calculations by not checking to see if the cell is truncated by the boundary of a higher-level cell [as suggested by Paul Goldhagen, Department of Energy (DOE)/Environmental Measurement Laboratory].

3.5.5. Warning for Bad WWINP File

The weight window values in superimposed mesh weight windows must be positive. If they are erroneously written with negative values (WWG card) or read from a WWINP file with negative values, a fatal error is issued. Otherwise, the run will proceed and later crash for mysterious reasons (as suggested by Paul Bailey, DOE/EML).

3.5.6. Print All Warnings to Screen

All warning messages, not just the first 20, now are printed to the terminal screen.

4.0. MCNPX 2.5.e CORRECTIONS

4.1. Significant Problem Corrections

The following problems could cause incorrect answers. Fortunately, they occur only in very special situations and affect only a few MCNPX users.

4.1.1. INCL4/ABLA Numerical Problems

The INCL4/ABLA physics package introduced in MCNPX 2.5.d is an event model developed in Europe by J. Cugnon (University of Liege, Belgium) and K. H. Schmidt (GSF, Darmstadt, Germany), in collaboration with J. C. David (CEA-Saclay, France) and others. To our knowledge, this is the first major widespread use of INCL4/ABLA in a general-purpose radiation transport code. Consequently, small errors that do not adversely affect single events can build up when the event estimator is called repeatedly for a random walk. MCNPX users of MCNPX 2.5.d observed crashes resulting from negative square roots, divides by zero, and other problems. These problems were caused by direction cosines not normalized perfectly and by very low energy particles (in kilo-electron volts). The corrections in MCNPX2.5.e check for negative square roots and zero divides and do not bank particles with energies less than 1 keV. Cash awards were made to Richard J. Olsher, LANL HSR-4 (D-5:JSH-2003-109) and Robin Klein Meulekamp, NRG, Petten, Netherlands (D-5:JSH-2003-112).

The INCL4/ABLA package now uses double precision for all variables and uses the MCNPX random number generator for all random numbers. One consequence of using the MCNPX random number generator is that calculations for N particles agree, whether they are done in a single run or in several continue runs. Also, debugging is easier because the Nth history can be restarted (DBCN card) and reproduced exactly as in a longer run.

The ABLA fission evaporation model now works correctly with the Bertini and ISABEL intranuclear cascade models, as well as with the INCL4 model.

J. C. David (CEA-Saclay, France) also has provided corrections to the spectrum at low energy. The bug was a bad determination of the emitted particle kinetic energy in ABLA for low excitation energies.

4.1.2. Spontaneous Fission as a Multiple Source Particle

When spontaneous fission was used as a multiple source particle and a spontaneous fission resulted in zero fission neutrons, transport of subsequent nonspontaneous fission source particles was omitted until the next spontaneous fission was sampled with one or more spontaneous fission neutrons. When this was a problem, the neutron summary table did not balance. An award of $20 was made to Martyn T. Swinhoe, LANL NIS-5 (D-5:JSH-2003-110).

4.1.3. Spontaneous Fission MCTAL Files

The normalization of tallies in MCTAL files for problems with spontaneous fission sources was the number of histories requested, not the number of spontaneous fission neutrons.

4.2. Irritating Problems

The following problems do not cause incorrect answers. In some cases, MCNPX will crash, and in others, the desired functionality simply is absent.

4.2.1. Periodic Boundaries Failed with Unused Surfaces

No previous MCNP/MCNPX versions eliminated unused macrobody facets or unused identical surfaces. In some cases, these unused surfaces would cause periodic boundaries to hit a fatal error for being bounded by a cell of nonzero importance. These unused surfaces now are eliminated, and the elimination of all unused or duplicate surfaces is more efficient. A $2 cash award was made to Adam Libal, Westinghouse, Sweden (D-5:JSH-2003-111).

4.2.2. MPI Load Balancing

The buffer ID was reset erroneously if the same host that ran the previous microtask also ran the current microtask. In very rare cases (with only a few CPUs), the buffer ID would be wrong and the code would crash.

4.2.3. MX Cards with Unused Materials

A fatal error occurred if an MX card were specified for a material not used in the problem. Now if an MX card is specified for an unused material, the MX card simply is ignored. A $2 award was made to Paul Bailey, Argonne National Laboratory (D-5:JSH-2003-114).

4.2.4. Mesh Tally Crash

Mesh tallies crashed in some cases if dumping to RUNTPE and printing (first two entries on PRDMP card) were different because the tally normalization was not yet set. A $2 award was made to Ian Smith, University of Liverpool, United Kingdom (UK) (D-5:JSH-2003-115).

4.2.5. PTRAC Cell/Surface Numbers with Flagging

PTRAK cell/surface numbers were wrong with cell/surface flagging. A $2 award was made to Valery Taranenko, GSF, Germany (D-5:JSH-2003-127).

4.2.6. Surface Transformations with Macrobodies

When surface transformations (TR cards) are used in conjunction with macrobodies, the SCF array can sometimes overflow, leading to a crash. A $2 award was made to Kin Yip, Brookhaven National Laboratory (D-5:JSH-2003-148).

4.2.7. Weight Window Generator for Charged Particle*s*

The weight window generator (WWG) card failed to write readable WWOUT/WWINP files in some cases for particle types IPT > 7. A $2 award was made to Ken Burn, ENEA, Bologna, Italy (D-5:JSH-2003-149).

4.2.8. User Error Crashing PC

If a user specifies an invalid ZAID such as zzzaaa.nnCC, the extra C can cause a memory leak; this caused a crash on a Windows PC system. A $2 award was made to Paul Goldhagen, USDOE/EML, New York (D-5:JSH-2003-128).

4.2.9. Infinite Loop for Different Time Cutoffs

If different time cutoffs are specified for different particle types, the code could go into an infinite loop. A $2 award was made to Fan Lei, QinetiQ, Farnborough, UK (D-5:JSH-2003-154).

4.2.10. GRIDCONV Crash if Max Contour >10

GRIDCONV would crash, put energies out of order, or get wrong file names if the maximum contour was greater than 10. A $2 award was made to Seiki Ohnishi, National Maritime Research Institute, Japan (D-5:JSH-2003-159).

4.2.11. Premature Termination for Electrons below Energy Cutoff

In rare cases, electrons falling below the electron energy cutoff could cause an EXPIRE termination with the error message "wrong material number." A $2 award was made to Yuri Franken, Eindhoven University of Technology, Netherlands (D-5:JSH-2003-163).

5.0. FUTURE WORK

- Pulse-height tallies with variance reduction
- Mesh tally contour plotting
- Cinder90 capabilities
    - Delayed neutrons physics models
    - Delayed gamma physics models
    - Transmutation
- Criticality
    - Externally driven sources
    - Improved stability of eigenfunctions
- Plotting of physics model total and absorption cross sections
- Forced collisions for neutral particles extended to physics models
- Improved high-energy physics with the LAQGSM model
- Secondary particle angle biasing for isotropic distributions
- Neutral particle perturbation techniques extended to physics model region
- Heavy-ion tracking and interactions
- Detectors and DXTRAN for all neutral particles at all energy ranges
- A capability to continue runs that write HTAPE files
- Interactive tally and cross-section plotting
- Integration of HTAPE tallies directly into MCNPX
- CAD link
- Magnetic field tracking